

Quantitative Determination of CL-20 Polymorphs by Mid-infrared Diffuse Reflectance Spectroscopy

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Abstract: The quantitative calibration models of three polymorphs α -CL-20, γ -CL-20, ε -CL-20 in ε -CL-20 product were established by mid-infrared diffuse reflectance spectroscopy combined with partial least squares (PLS) method of chemometrics, and the cross-validation and external validation to the models were performed. Results show that three models have high accuracy and precision, the determination coefficients of cross-validation (R^2) are 0.9973, 0.9714, 0.9848, respectively, and the root mean square error of cross-validation (RMSECV) are 0.222%, 0.650%, 0.670%, respectively. In the external validation, the root mean square error of prediction (RMSEP) are 0.422%, 0.813%, 1.02%, respectively, and the paired *t*-test results show that there is no significant difference between predicted values and actual ones. The quantitative analysis method of CL-20 polymorphs based on the above models can be applied to the product quality test of ε -CL-20, and the studies on the polymorph stability of ε -CL-20 in technical process and long-time storage of explosives and propellants.

Key words: CL-20; quantitative analysis of polymorph; mid-infrared diffuse reflectance spectroscopy; partial least squares (PLS) method

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